Modeling Block Copolymer Interactions with Biomimetic Membranes

Scientific Achievement

A coarse grained model for molecular dynamics simulations of polymer lipid-based systems has been developed. This reduced model retains close connections to the underlying atomistic representation while extending the simulation timescales to nanoseconds or more, a necessary approach for the study of large molecule diffusion in bilayers. The molecular dynamics simulations have shown that the mode of insertion, harpoon or spanning, depends on the hydrophobic block length of triblock copolymers. A hydrophobic segment of greater or equal to 12 coarse grained beads (36 PPO units) will fully insert into the lipid bilayer. Smaller lengths of the hydrophobic block will preferentially promote the polymer to adopt a harpoon configuration. Simulation results are compared to experimental studies.

Small Angle X-ray Scattering (SAXS) studies on PEO-PPO-PEO triblock-DMPC system indicate that when the hydrophobic block (PPO) length is much smaller compared to the bilayer thickness, the copolymer is in a harpoon configuration with both hydrophilic segments on the same side of the bilayer. On the other hand, when the hydrophobic segment length is large enough, the triblock can insert completely such that the two hydrophilic segments are on the opposite sides of the bilayer. This configuration can be used to modify such bilayer properties as bending modulus and interlamellar distance.

Significance

Understanding the interaction between block copolymers and biological membranes on the molecular level is crucial for the design of molecular therapeutics used to treat soft tissue injuries and for the rational design of new soft materials. Association of block copolymers such as PEO-PPO with phospholipid based complex fluids results in versatile novel materials with enormous potential in many areas of bionanotechnology and nanomedicine. The molecular architecture and concentration of block copolymers along with environmental variables such as temperature and pH provide means to tune these structures for desired applications and also allow for designing signal-responsive materials. MD simulations along with experimental techniques can explore the effects of molecular architecture and concentration on the phase behavior of these materials. In particular, the harpoon configuration of triblock copolymer studied in this work is ideal for sealing defects in cell membranes with a potential for new approaches to healing and repair disrupted cellular structures.

Performers

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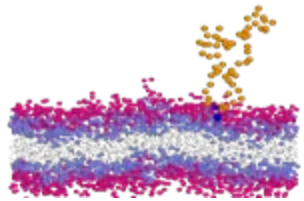
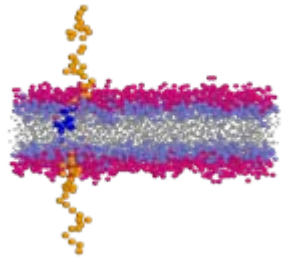
Modeling Block Copolymer Interactions with Biomimetic Membranes

Objective:

Understand the physics behind block copolymer-lipid association and develop new approaches to design of bionanostructures.





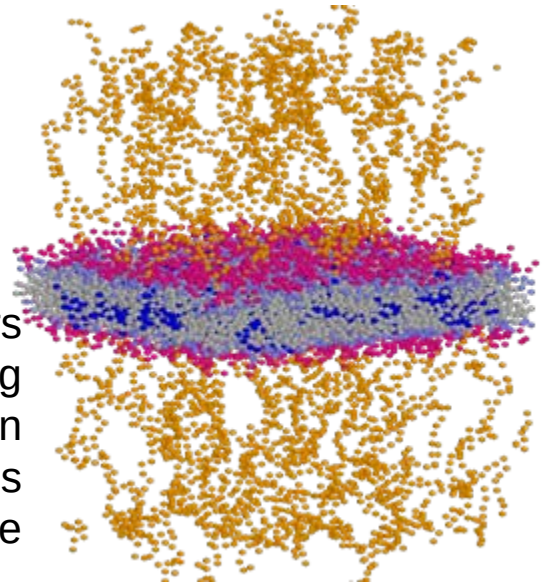
Harpoon Spanning

Accomplishments

Developed coarse grained model for molecular dynamics simulations of polymer lipid systems.

Found the dependence of the mode of insertion, harpoon or spanning, on hydrophobic segment length of triblock copolymers.

Small Angle X-ray Scattering results on triblock-DMPC bilayers are in agreement with the simulations.



Future work:

The effect of concentration and architecture of block copolymers on the phase behavior of lipid bilayers will be investigated using simulations and mean field theory. These studies will result in understanding the rich phase diagram of these complex fluids and will lead to rational design of new soft nanoscale architectures.

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